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Metastable states and information propagation in a 1D array of locally-coupled bistable cells

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Abstract

We study the effect of metastable states on the relaxation process (and hence information propagation) in locally coupled and boundary-driven structures. We first give a general argument to show that metastable states are inevitable even in the simplest of structures, a wire. At finite temperatures, the relaxation mechanism is a thermally assisted random walk. The time required to reach the ground state and its life time are determined by the coupling parameters. These time scales are studied in a model based on an array of quantum dots.

A number of novel proposals have recently been advanced, articulating primarily, visions of future computing systems [1–7] using nanoelectronic structures [8–10], in which computation is fundamentally related to the underlying physics of the devices. In this paper, we consider one such class of models comprising of an array of locally-coupled and edge-driven cells, where computation is realized by relaxation of the physical system to its ground state [1–3]. These models are semiclassical and global phase coherence is not maintained as the system relaxes to its ground state by dissipative processes.

The computing architecture comprises of locally-coupled arrays of a basic unit that exhibits bistability and the bistable states are used to represent the binary values 0 and 1 (Fig. 1(a)). The basic units interact with their nearest neighbors to form larger devices such as wires, logic gates and cellular automata (Fig. 1(b)) [2,3]. The units on the edges form the input and output ports (Fig. 1(b)), and the interior units of the device are not externally accessed [2,3]. Both information and energy are provided to these boundary ports as input data. *Central* to the operation of the computing system is the assumption that the system then relaxes by dissipation to the ground state that depends only on the configuration of the input cells, which are held fixed. The ground state configuration represents the result of the computation and the output is read from the cells marked 'output' (Fig. 1). For example, consider a wire which consists of a linear array of basic units as shown in Fig. 2(a). The ground state is two fold degenerate; all cells have a bit value of either 0 or 1 (Fig. 2(b)). Computation is based on the thesis that the system always relaxes to the ground state determined by the bit value of the input cell, thus transmitting information from the input to the output of the wire.

The proposed models, which involve a Hubbard-type Hamiltonian clearly demonstrate that the ground state of suitably designed structures correspond to computationally useful operations [2,3]. While this is an important first step, it is essential to study the dynamical evolution of the computational trajectory because it is a priori not clear that the system will in fact relax to the ground state ever, or, in a time efficient manner. Our specific concern is metastable states, which may hinder relaxation to the ground state as hypothesized in Refs.

[11] and [12].

In the first part of the paper, we will give a simple insightful argument as to why metastable states are inevitable in a wire. As a consequence of the metastable states, information propagation is not feasible at extremely low temperatures. The computing system can however escape from the metastable states and reach the ground state at non zero temperatures via a thermally assisted random walk; thus propagating information from the input to the output end of the wire. A discussion of this in the context of a model comprises the second part of the paper.

Consider the initial state of a wire with bit value 0 in the input cell and bit value 1 in the remaining cells (Fig. 2(a)). The intersection of the left and right aligned cells is referred to as a *kink*. If the system relaxes to the ground state as time evolves, it is expected that the kink will propagate towards the right, into the bulk of the wire. The state where the kink is m units from the input end is denoted by ϕ_m and its energy is denoted by $E(m)$ (Fig. 3(a)). The computational trajectory from ϕ_m to ϕ_{m+1} may in principle involve many intermediate states but for simplicity we will assume that there is only a single intermediate state which is denoted by ϕ'_m and its energy is denoted by $E'(m)$. In a long wire, states ϕ_m and ϕ_{m+1} have almost the same energy because their left and right environments are nearly the same. As a result, the total energy versus state of the system should vary periodically in the bulk as shown in Fig. 3(b). ϕ_m is a metastable state because the $\phi_m \rightarrow \phi'_m$ and $\phi_m \rightarrow \phi'_{m+1}$ transitions require surmounting of energy barriers in the bulk (ΔE). Note that in principle the energies of the primed and unprimed states could be interchanged, in which case the primed states will be the metastable states.

Varying the inter and intra cell interactions yields different values of the ΔE. However, even for parameters where ΔE is close to zero, we argue that metastable states should exist at least either near the left or right edges. The cells close to the edges have a non symmetric environment to its left and right. As a result, ΔE will be non zero near the edges. If $E'(1) > E(1)$, then trivially the initial state is a metastable state. If not, then by symmetry of the structure $E(N-1) > E'(N-2)$ and this results in a metastable state (N is the

total number of cells in the wire). It should also be noted that in a structure where ΔE is designed to be zero, small undesired fluctuations in the inter and intra cell interactions cause $E(m) \neq E(m+1)$, leading to metastable states [12].

We have shown that metastable states exist at zero temperature. At finite temperatures, the kink propagates to the right via a thermally assisted random walk, where the various states, accessed (Fig. 3) from the input end to the output form the lattice points. Note that the thermally assisted random walk is the only mechanism to overcome any ΔE since there are no fields driving the computation. The probability to hop from the lattice point representing state ϕ_m to the lattice points representing ϕ'_m and ϕ'_{m-1} are given by $\Gamma_{\phi_m \rightarrow \phi'_m}/(\Gamma_{\phi_m \rightarrow \phi'_m} + \Gamma_{\phi_m \rightarrow \phi'_{m-1}})$ and $\Gamma_{\phi_m \rightarrow \phi'_{m-1}}/(\Gamma_{\phi_m \rightarrow \phi'_m} + \Gamma_{\phi_m \rightarrow \phi'_{m-1}})$ respectively, where $\Gamma_{a \rightarrow b}$ is the transition rate to go from state a to state b. A similar expression applies for the transition probabilities from ϕ'_m to ϕ_m and ϕ_{m+1}. For a uniform and long wire, these transition probabilities are equal to one half, when ϕ_m represents a state where the signal (kink) has traveled into the interior of the wire. This is because the energy differences $E'(m) - E(m)$ and $E'(m-1) - E(m)$ are nearly the same. The random walk is a finite one with an absorbing boundary on the right end (the walk stops when the output is reached) and a reflecting boundary on the left end (signifies that the input cell has a fixed state). The average time taken for the signal to propagate from the initial state to the ground state (T_{tot}) is the quantity of interest. We are not aware of analytical techniques to calculate T_{tot}. However, to understand the underlying physics, it is useful to consider the time required for the kink to travel n cells in the bulk of a wire (i.e. edge effects are not included). This time follows directly from the discussion of random walk [13] and is,

$$\text{Time required to travel } n \text{ cells} \sim (2n)^2 \, \frac{\tau_1 + \tau_2}{2} \, , \tag{0.1}$$

where, τ_1 and τ_2 are the life times of the metastable states and the states in between two consecutive metastable states (Fig. 3). The factor $2n$ represents the fact that there are two states involved in the propagation of the signal across each of the n cells. At low temperatures ($kT < \Delta E$), the time in Eq. (0.1) is primarily determined by $\tau_1 \sim \tau_0 exp(\Delta E/kT)$, where

τ_0 and ΔE, the energy barrier of the metastable states encountered in the bulk (Fig. 3), depend on the particular model. From the exponential dependence of τ_1, it is clear that T_{tot} increases exponentially with decrease in kT. T_{tot} can be made smaller by raising the temperature. The temperature, however, cannot be increased indefinitely because for the computation to be useful, the system must remain in the ground state for a long enough time so that we know for certain that the ground state has been reached and that the system has not escaped from it. The life time in the ground state varies with temperature as $\tau_g exp(\Delta E_g/kT)$, where τ_g and ΔE_g (the energy barrier separating the ground state and the next excited state that can be reached) are constants. To realize a computation, it is important that the temperature is large enough to shake the system out of a metastable state but not so large as to excite the system out of the ground state in a short time period. Hence, it is necessary that the energy difference between the ground state and the excited states (which are reached by a single electron tunneling event from the ground state) is many times the thermal energy kT and the energy barrier due to metastable states is comparable to or smaller than kT. The relative magnitudes of ΔE, ΔE_g and other energy barriers close to the edges are determined by the device parameters. It is essential to determine if there exists a region in the parameter space of the device dimensions and temperature, where the system relaxes to the ground state quickly and also remains there for a sufficiently long time period to be computationally useful. We study this by considering the time evolution of a specific model.

The model considered is one similar to that discussed in the literature before [14]. The basic unit consists of four identical metallic type quantum dots containing a net charge of two electrons. A wire is comprised of a linear array of these units (Fig. 4). The tunnel resistance between the dots is much larger than h/e^2. In this limit, each dot contains an integer number of electrons. The intra and inter cell interactions are modeled by capacitances C and C' respectively. C_0 is the capacitance between a dot and the ground. The values of these capacitances do not vary from cell to cell. The tunnel resistances between the dots along the sides of a single cell are represented by R and the tunnel resistances between dots

along the diagonals of a cell and between dots of different cells are infinite. Though imaging of charge to the outside world is unavoidable, models for ground state computing have neglected this feature all together. The total energy of a charged system without imaging to the outside world (i.e., $C_0 = 0$) is infinite and so we have to assume at least a small value for C_0 in the calculations. We have chosen $C_0 = 0.001C$ throughout this paper.

In the lowest energy state, the two excess electrons in an isolated cell are aligned either along the left or right diagonals and these two states represent the binary values 0 and 1. The ground state of the wire is two fold degenerate as shown in Fig. 2(b).

The time evolution is modeled by the orthodox theory of single electron tunneling [15], where the transition rate for a single electron tunneling event from dot i to dot j is,

$$\Gamma_{ij} = \frac{\Delta E_{ij}}{q^2 R} \frac{1}{exp(\Delta E_{ij}/kT) - 1}, \tag{0.2}$$

where R is the tunnel resistance between dots i and j. $\Delta E_{ij} = E_a - E_b$, where E_a and E_b are total energies of the system after and before the tunneling event. Using the standard monte carlo method as applied to single electron tunneling [16], we compute the time taken to reach the ground state (T_{tot}) as a function of the temperature for wires of various lengths, with the initial states as shown in Fig. 2(a). The main results of this simulation are summarized in Fig. 5(a). As the temperature tends to zero, T_{tot} tends to infinity and the ground state is never reached (this is not strictly true if *higher order* quantum mechanical co-tunneling processes are included). At small temperatures, where kT is much smaller than all barrier heights encountered in the computational trajectory, T_{tot} decreases exponentially with increase in temperature. This can be understood by noting that the various tunneling probabilities depend exponentially on $\Delta E/kT$, where ΔE is the barrier that an electron should surmount to overcome a metastable state (Eq. (0.2)). At temperatures comparable to or larger than ΔE, T_{tot} decreases inversely with temperature. This can again be understood from Eq. (0.2) because for $kT > \Delta E$, $\Gamma_{ij} \propto T^{-1}$. The temperature however cannot be made very large because the life time of the system in the ground state decreases with increase in temperature and this is undesirable for computing. The largest temperatures chosen in Fig.

5(a) is $0.075e^2/C$, which is larger than ΔE_g (Fig. 3). Even at this temperature, which is not suited for ground state computing, the time taken to reach to ground state is too large; it takes $10^5 RC$ for the system to reach the ground state of a wire with only sixty cells. A value of $C'/C = 1.3$ was chosen for these simulation. We have performed simulations for other parameters and find that the results are not significantly different. Though Eq. (0.1) was not intended to calculate T_{tot}, we remark that substituting $n = 60$ and the appropriate values for kT and ΔE in Eq. (0.1) gives a time which agrees with T_{tot} to about an order of magnitude.

To see that there is only a narrow region of capacitance parameters and temperature where the system relaxes to the ground state and remains there for long times, we plot ΔE and ΔE_g versus C'/C in Fig. 6. Here, for $C'/C \geq 2.1$, $|\Delta E| \geq |\Delta E_g|$. This leads to a shorter life time in the ground state than in the metastable states and is therefore undesirable for computing. For $C'/C \leq 1$, the magnitude of $|\Delta E_g| - |\Delta E|$ decreases as C'/C becomes smaller. As a result, the temperature of operation has to be made correspondingly smaller to ensure that the life time in the ground state is significantly larger than the life time in the metastable states. However, T_{tot} increases exponentially with decrease in temperature and so very small values of C'/C are also undesirable. Fig. 6 is a plot of only two types of metastable states, the ones in the bulk of the wire and ΔE_g. Other metastable states close to the edges of wire play an important role too, especially for small values of $|\Delta E|$.

Finally, we address the issue of how the system evolves to the ground state: A wire with N cells has $8(N-1)$ possible transitions which compete to determine the state of the wire in the next time step. In the discussion surrounding Fig. 3, we assumed that the cells flip from the left (input) to the right end in a specific manner such that a single kink performs a thermally assisted random walk. We find from our monte carlo simulations that this picture is valid: having more than one kink is energetically expensive and each cell flips from a left to a right aligned one (or vice versa) via the path shown in Fig. 5(b).

We have also performed simulations on a fanout gate [2,3], which comprises of a single input, which is transmitted to two output ports (Fig. 7). The metastable states that have

to be overcome here are far worse and an intuitive reason is as follows. The polarization of Cell 2 can flip as in the case of a wire. For the signal to propagate further, it is essential for Cell 3 to flip its polarization. Cell 3 has two neighbors (4 and 7) which have the same polarization and one neighbor (Cell 2) with the opposite polarization. It is however energetically unfavorable for Cell 3 to flip because the new state would have two kinks, thus resulting in a far worse metastable state than in the case of the wire. In summary, we have shown that metastable states always exist in locally-coupled edge-driven computing systems, thus preventing information propagation at very low temperatures. At finite temperatures, relaxation to the ground state and hence propagation of information along the wire takes place by the inefficient process of a thermally assisted random walk.

Note: We would also like to bring to notice a recent proposal [17] for computing which uses bistable cells evolving under the presence of a spatially and adiabatically time varying field. The physics of such systems are different from that discussed here.

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FIGURE CAPTIONS:

Fig. 1: (a) A single bistable cell: the lines along the left and right diagonals represent the binary values 0 and 1. (b) schematic of a corresponding computing system.

Fig. 2: (a) The initial state and (b) the two degenerate ground states of the wire.

Fig. 3: (a) State ϕ_m, where the signal has transmitted m cells deep into the wire. (b) A qualitative plot of the energy versus the states accessed as the signal propagates away from the edges of the wire.

Fig. 4: (a) Electrons occupying diagonally opposite dots represent binary values of 0 and 1. (b) A wire constructed from the basic units in (a).

Fig. 5: (a) Time taken to reach the ground state versus temperature for wires of different lengths ($C'/C = 1.3$) (b) Sequence of steps by which the polarization of a cell flips.

Fig. 6: A plot of $|\Delta E|$ (solid line) and $|\Delta E_g|$ (dashed line) discussed in the context of Fig. 4 versus C'/C.

Fig. 7: Fanout gate